

Ethane, methoxy-d3  
16995-14-5 | DTXSID20168777

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $5.09\text{e-}12 \text{ cm}^3/\text{molecule}\cdot\text{sec}$

**Global applicability domain:** Inside

**Local applicability domain index:**  $7.80\text{e-}01$

**Confidence level:**  $5.54\text{e-}01$

## Nearest Neighbors from the Training Set

[Image not found](#)

Tetrahydrofuran

**Measured:**  $1.61\text{e-}11$

**Predicted:**  $7.41\text{e-}12$

[Image not found](#)

Diethyl ether

**Measured:**  $1.31\text{e-}11$

**Predicted:**  $9.74\text{e-}12$

[Image not found](#)

1,2-Propylene oxide

**Measured:**  $5.20\text{e-}13$

**Predicted:**  $2.37\text{e-}12$

[Image not found](#)

1,3-Propylene oxide

**Measured:**  $1.03\text{e-}11$

**Predicted:**  $6.49\text{e-}12$

[Image not found](#)

1,2-Epoxybutane

**Measured:**  $1.91\text{e-}12$

**Predicted:**  $5.74\text{e-}12$